Quasi-one-dimensional Peierls dielectric in a constant electric field

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The behavior of a Peierls dielectric (PD) with a doubled period in a uniform electric field is investigated within the framework of the microscopic approach. It is shown that the electric field suppresses the gap Δ_0 in the conduction-electron spectrum and creates pairs of free carriers by tunneling. The latter process ensures in fields $eE_c \sim \Delta_0 \xi_0^{-1} (\xi_0 = \hbar v_F/\Delta_0)$ a smooth transition of a PD into the metallic phase. Temperature effects in PD are considered.

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INTRODUCTION

Experimental and theoretical studies of quasi-one-dimensional compounds that undergo a metal–insulator Peierls transition have attracted much interest recently. It is known that the Peierls transition is accompanied by lattice-structure changes and by the onset of an energy gap in the electron spectrum. This gap separates the filled electronic states from the conduction band. Below the transition point, the dielectric state is characterized by a microscopic lattice displacement

$$u(x) \sim \bar{\Delta} \cos (2k_F x + \varphi),$$

where k_F is the Fermi momentum, $\bar{\Delta}$ determines the gap in the carrier spectrum, and the phase shift $\varphi(x,t)$ characterizes the charge-density wave.

The thermodynamics of the Peierls transition in the absence of external field was considered by many workers (see, e.g., the reviews[1]). In later studies[2-8] it was noted that there can exist in the Peierls phase nontrivial conduction mechanisms connected with soliton-type collective excitations in the electron-ion system.

The simplest type of Peierls transition is a phase transition with doubling of the period. In this case the Peierls shift $u_n \sim (-1)^n \Delta$ and there is no phase degree of freedom.[1] According to present notions, such a situation is possibly realized in chains of polyacetylene $(CH)_x$.[6] When not doped, $(CH)_x$ is a semiconductor with a large energy gap $\Delta \sim 1$ eV. However, even a weak ($\sim 0.5\%$) doping of the polyacetylene leads to a noticeable conductivity, due apparently to the appearance of free large-radius polarons. These polarons constitute each a bound state of an electron and a lattice soliton.[2,7,8] Favoring this assumption is the large conductivity of doped $(CH)_x$ with complete absence of Pauli magnetic susceptibility of the free carriers[9] in a large range of doping densities.

In connection with the observed anomalous properties of the conductivity of $(CH)_x$ (Refs. 6 and 9), great interest attaches to the development of a consistent microscopic theory of the behavior of a Peierls dielectric (PD) with doubling of the period in an external electric field E at a finite temperature T. This question was first considered in Ref. 10, where it was shown that the influence of a constant external field leads to suppression of the gap in the PD spectrum, and in final analysis to the restoration of the metallic state. This conclusion was based on an analysis of the thermodynamics of PD in an external field E. In the present paper, within the framework of the microscopic approach, we analyze in detail the mechanism of the destruction of a PD in an electric field. The electric field plays a twofold role in the Peierls phase. First, it decreases the energy gap[10] (the effect of polarization of the PD). Second, a probability of tunnel formation of (particle-hole) pairs of free carriers appears even in arbitrarily weak electric field.[11] Whereas the first aspect of the action of the field on the PD can be treated within the framework of thermodynamics, the processes of pair production from the ground state of the PD (vacuum) is of purely dynamic origin.

A consistent theory of a PD in an electric field should include a detailed analysis of the dynamics of the free carriers in the conduction band (of the holes in the valence band). There are two limiting cases here. It is known (see, e.g., Ref. 12) that in the absence of scattering mechanisms the motion of the charge in the band is finite and periodic, with a spacial period $L_{band} \sim \hbar v_F/eEa$ (v_F is the Fermi velocity, a is the lattice constant, and e is the electron charge). The field does not lead in this case to formation of direct current, and the PD, despite the production of carrier pairs, remains in this sense an insulator (the high-frequency conductivity, naturally, differs from zero).

For organic quasi-one-dimensional compounds it is the opposite limit which is realized, with the mean free path much less than L_{band}. The produced free carriers produce in this case a direct current. This is precisely the situation investigated in the present paper. The nonstationary character of the behavior of PD in an electric field, due to the instability of the

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vacuum, does not make it possible to employ the thermodynamic approach in the entire range of electric fields and temperatures. Therefore at the parameter values at which the effects of particle production from vacuum become of the same order of magnitude as the polarization effects (strong nonstationarity), the very concept of a thermodynamic phase transition becomes meaningless, and the restoration of the metallic state proceeds smoothly (without singularities in the kinetic coefficients).

Free charges in PD at equilibrium exist in the form of solitons of the order parameter

$$\Delta(x)=\Delta_0 \operatorname{th}(x/\xi_0),$$

where Δ_0 is the equilibrium gap and $\xi_0=\hbar v_F/\Delta_0$ (Refs. 2 and 6–8). The formation of a soliton is due to the interaction of the two subsystems that make up the PD: rapid electronic ($t_e \sim \hbar/\Delta_0$) and slow lattice $[t_L \sim \lambda^{-1/2}/\omega(2k_F)]$ subsystems, where $\lambda=g^2/\pi\hbar v_F$, g is the electron-phonon interaction constant, and $\omega(2k_F)$ is the frequency of the bare phonons with momentum $2k_F$ (Ref. 1). The ratio $(t_e/t_L)^2=\alpha^2 \ll 1$ ensures applicability of the self-consistent-field theory to the description of the PD at low temperatures.[2] The soliton energy $E_s=2\Delta_0/\pi$ (Ref. 13 and 2) is determined by the contribution of the fast electronic processes, and its mass M_s is connected with the inertia of the lattice, $M_s \sim E_s/(\alpha v_F)^2$.

An electric field E introduces into the problem new time scales that characterize the charge production by tunneling

$$t_E^{e,s} \sim \hbar/eE\lambda\!\!\!^{-}{}^{e,s},$$

where $\lambda\!\!\!^{-}$ is the Compton wavelength, with $\lambda\!\!\!^{-}{}^e=\xi_0$ for electrons and $\lambda\!\!\!^{-}{}^s=\alpha\xi_0$ for solitons. In a large field interval $\alpha^2E_c<E<E_c$, $E_c\sim\Delta_0^2/\hbar e v_F$, and $T_E^e<t_L$, so that tunnel production of free electron-hole (e-h) pairs takes place at a fixed lattice configuration $\Delta=\Delta_0$. This makes it possible to consider, in the field interval indicated above, the effects of production and polarization of the ground state of the PD at the electron level. The soliton character of the carriers manifests itself, of course, in the calculation of the mobility in the steady-state conduction regime. It was precisely under such physical conditions that we have formulated and investigated the model of a PD in an external field at low temperatures. The low temperature means that a free-carrier density is ensured completely by the tunnel decay of the ground state of the PD in the electric field and the characteristic energies of the particles in the field are $eE\hbar v_F/T \gg T$.

An entirely different situation takes place at thermodynamic equilibrium, when the equilibrium densities of the particles and their kinetic energies are governed by the temperature ($eE\hbar v_F \ll T^2$). It is clear from the foregoing that for PD with double the period there can be no free electrons and holes at equilibrium. Therefore the thermodynamics of PD at $T\ll\Delta_0$ (this condition is always satisfied in real quasi-one-dimensional systems, since the temperature of the three-dimensional ordering turns out to be much lower than Δ_0, Ref. 1) should be based from the very outset on the treatment of solitons as quasiparticles of a one-dimensional Peierls chain.

The nonzero density of the order-parameter solitons at nonzero E and T means formally the absence of long-range order in the one-dimensional system.[14] At $T\ll\Delta_0$ and $E\ll E_c$, however, their density is exponentially low and one can speak of a one-dimensional PD and of a rarefied soliton gas in it. It behooves us here to analyze in greater detail the concept of a homogeneous PD in an electric field. Let us imagine that the field penetrates into the Peierls chain inhomogeneously, forming a periodic domain structure. The energy of such a structure (with allowance for the field energy) exceeds the energy of the homogeneous state. Indeed, the energy gain in the presence of a field is connected in final analysis with the increase of the dielectric constant ε. This gain can always be realized by decreasing Δ uniformly. In the upshot the inhomogeneous structure experiences a net loss of energy, due to the Δ gradients. This situation differs in principle from type-II superconductors, where the magnetic field stabilizes the inhomogeneous structure of the order parameter.

In this paper we construct a microscopic model of a homogeneous PD with doubling of the period in an external electric field at finite temperature. Within the framework of the method of functional integration, using the formalism of the generalized ζ function, we consider the effects of polarization of the ground state of the PD and of production of free carriers. We obtain for $T=0$ an exact expression for the real and imaginary parts of the ground-state energy, and also calculate the temperature corrections in the region where the temperature is low compared with the characteristic energy of the pair produced in the field E. The thermodynamic description becomes possible in the opposite limit, where the temperatures are high compared with this energy. The equilibrium value of the gap Δ is determined in this case by the temperature, and small field corrections account for the weak violation of the thermodynamic equilibrium. The Appendix contains the necessary mathematical formulas that arise in the calculation of the functional determinants by the generalized ζ-function method.

MICROSCOPIC MODEL OF PEIERLS DIELECTRIC WITH DOUBLED PERIOD IN AN ELECTRIC FIELD

The microscopic treatment of the PD is traditionally based on the Fröhlich Hamiltonian, in which the normal coordinates of the lattice with wave vector $q=2k_F$ are replaced by mean values. Following the standard procedure (see, e.g., Refs. 15 and 16), we write the Hamiltonian in the form

$$H=\frac{\Delta^2}{g^2}+\sum_\sigma\left\{\hbar v_F\bar{\Psi}_\sigma\sigma_2\frac{\partial}{\partial x}\Psi_\sigma+\Delta\bar{\Psi}_\sigma\Psi_\sigma\right\}. \tag{1}$$

Here σ is the electron spin, $\bar{\Psi}=\Psi_\sigma^+\sigma_3$, and σ_i are Pauli matrices. We recall that the following simplifications were made in the derivation of (1): the dispersion law of the bare electrons was normalized near $k=k_F$ $[\varepsilon(k)\approx v_F(k-k_F)]$, and the lattice kinetic energy

$$H_{\text{kin}}=\Delta^2/g^2\omega^2(2k_F) \tag{2}$$

was left out. The term (2) determines the quantum fluctuations of the field Δ, which are small in the parameter $\alpha^2 \ll 1$. It will therefore not be taken into account in the calculation of the ground-state energy of the PD (the adiabatic approximation).

The constant electric field $A_\mu = (0, -Et)$, $\mu=1, 2$ is included, as usual, by lengthening in (1) the derivative $\partial/\partial x \to \partial/\partial x - ieA_2$. We shall find it convenient hereafter to change to the Lagrangian form of the PD model. According to (1), the density of the Lagrange function in an electric field is given by ($\hbar = v_F = 1$)

$$\mathscr{L}=\sum_\sigma \{i\bar{\Psi}_\sigma\gamma_\mu D_\mu\Psi_\sigma-\Delta\bar{\Psi}_\sigma\Psi_\sigma\}-\frac{\Delta^2}{g^2}, \tag{3}$$

where $D_\mu = \partial_\mu - ieA_\mu$ and $\gamma_\mu = (\sigma_3, i\sigma_2)$. The Lagrangian (3), which will hereafter be the starting point in our calculations, corresponds to the known Gross-Neveau model.[13,14,17]

Simple estimates show that in fields $E > \alpha^2\Delta_0^2/e\hbar v_F$ it is possible to disregard the soliton character of the carriers in the PD, and to analyze the influence of the electric field at the level of the Lagrangian of the bare electrons (3) ($\Delta = \text{const}$).

We proceed to calculate the energy of the ground state in the model (3). The complete solution of the problem consists of calculating the vacuum-vacuum amplitude in the presence of a source J that lifts the degeneracy $\tilde{\Delta} \to -\tilde{\Delta}$:

$$\exp(iW_J)=\int D\Psi D\bar{\Psi} D\tilde{\Delta}\exp\left\{i\int dx_\mu(\mathscr{L}+J\tilde{\Delta})\right\}. \tag{4}$$

At a temperature $T=0$, expression (4) determines the ground-state energy of the PD in the presence of an external field E. At $E=0$ and $T\neq 0$ Eq. (4), following the standard substitution $t \to -i\tau$, determines the partition function of the system, if the functional integral is calculated over periodic fields $\tilde{\Delta}$ (with period $\beta = 1/T$) and antiperiodic fields Ψ and $\bar{\Psi}$ (having the same period) (see, e.g., Ref. 18).

What happens to the system when simultaneous account is taken of the electric field and of the temperature? A temperature implies specified equilibrium densities of the stable excitations in the system (soliton-antisoliton pairs), and its influence in the absence of a field reduces only to a renormalization of the gap. Inclusion of the field leads to a distortion of the distribution functions, so that one can speak of thermodynamic equilibrium (i.e., of a temperature) only if the density of the nonequilibrium particles is low. (Temperatures higher in comparison with the characteristic energy of the pair in the field, $eE \ll T^2$.) In the other limiting case ($eE \gg T^2$), which is investigated by us, the dynamics of the system is determined mainly by the field, while the temperature describes small equilibrium fluctuations in each dynamic state.

Proceeding to specific calculations, a short remark is appropriate concerning the experimental setup for the study of the polarization of the PD in an electric field. It is known that a longitudinal field can act on the system in two ways (see Ref. 19). In one case the induction D (the charge on the capacitor plates) is specified and in the other the field E, which is determined by the potential difference. Bearing in mind the use of the calculations for a possible explanation of the nonlinear current-voltage characteristics of PD (see, e.g., Ref. 20), we shall consider the problem in the second formulation.

To calculate the energy of the ground state as a function of a homogeneous order parameter $\Delta(E, T)$ it is convenient to change from W to the effective potential[21]

$$V_{eff}(\Delta)=\left(-W+\int dx_\mu J\Delta\right)\Big/\int dx_\mu, \tag{5}$$

which has extremal properties with respect to Δ. The effective potential is a convenient quantity in the investigation of the properties of systems with spontaneous symmetry breaking. In a zero field and at zero temperature, $V_{eff}(\Delta)$ coincides with the energy of the ground state of the system with order parameter Δ, and at $T\neq 0$ the real part of V_{eff} determines at equilibrium the free energy of the system.[22,14]

For the model (3), recognizing that the field Δ is classical, and also integrating in (4) over the Fermi fields, we have[23]

$$V_{eff}(\Delta)=\frac{\Delta^2}{g^2}+\left(\int dx_\mu\right)^{-1} i\,\mathrm{Sp}\ln(i\gamma_\mu D_\mu-\Delta). \tag{6}$$

The trace symbol implies summation over the matrix indices and integration with respect to the coordinates. An effective method of calculating the functional determinant, whereby account is taken automatically of temperature effects, was proposed in Ref. 24 (see also Ref. 25). According to Ref. 24, the spare of the logarithm of the electric operator $\hat{M}_e$ is represented in the form

$$\mathrm{Sp}\ln\hat{M}_e\equiv\ln\mathrm{Det}\,\hat{M}_e=-\zeta'(0)-\zeta(0)\ln c_R^2, \tag{7}$$

$$\zeta(s)=\sum_n\lambda_n^{-s}, \tag{8}$$

where λ_n is the set of eigenvalues of the operator $\hat{M}_e$, and c_R is a normalization constant. To apply Eq. (7) in our case, we change over to imaginary time $t \to -i\tau$ and rewrite V_{eff} in the form

$$V_{eff}=\frac{\Delta^2}{g^2}+\frac{1}{L\beta}\{\zeta'(0)+\zeta(0)\ln c_R^2\}, \tag{9}$$

where $L\beta$ is the value of the two-dimensional space (in our case L is the length of the chain and $\beta = 1/T$).

Our problem was reduced to finding the eigenvalues of the operator $(i\gamma_\mu D_\mu - \Delta)_e$ and to their use to construct the generalized ζ function. It is most convenient to calculate $\zeta(s)$ using the eigenvalues of the quadratic operator

$$\hat{K}=-(i\gamma_\mu D_\mu-\Delta)_e(i\gamma_\mu D_\mu+\Delta)_e, \tag{10}$$

$$\ln\mathrm{Det}\,\hat{M}_e={}^1/_2\ln\mathrm{Det}\,\hat{K}. \tag{11}$$

Using the commutation properties of γ matrices in Euclidean space

$$[\gamma_\mu,\gamma_\nu]_+=-2\delta_{\mu\nu}, \tag{12}$$

we obtain

$$\hat{K}=-(\partial_\mu-ieA_\mu)^2+\Delta^2+{}^1/{}_2e\sigma_{\mu\nu}F_{\mu\nu},$$
$$\sigma_{\mu\nu}={}^1/{}_2i[\gamma_\mu,\gamma_\nu]_-,\quad F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu. \tag{13}$$

In Euclidean space (τ,x), E plays the role of the "magnetic" field H. In the later calculations we shall retain the symbol H until we make the transition to the (t,x) space in the final formulas, where $H\to -iE$.

The equation for the eigenvalues of the operator $\hat{K}$ is of the form

$$\left\{\frac{d^2}{d\tau^2}+\lambda_n-\Delta^2+e\mu H-(p_x-eH\tau)^2\right\}\Phi_n=0, \tag{14}$$

where p_x is the conserved momentum along the x axis and $\mu=\pm1$. Equation (8) is the known equation for the parabolic-cylinder functions. Thus, the transition to imaginary time reduces the problem to a calculation of the energy of a two-dimensional fermion in a magnetic field. Allowance for the presence of two bands means summation over the μ-projection of the "spin" of the two-dimensional electron. It is easily seen that (14) has exact periodic solutions only at $H=0$. Turning on the field disturbs the periodicity of the solutions (14). It is this which reflects formally the fact that the electric field violates the thermodynamic equilibrium.

Starting from the physical picture described earlier, we can determine the spectrum (14) in two asymptotic regions. We start with the case of a weak field. Equation (14) has an antiperiodic solution

$$\Phi_n\sim\exp\{i\pi(2n+1)\tau/\beta\}$$

under the conditions

$$|p_x|\gg eH\beta,\ eH\beta^2\ll1,\ eH\ll\Delta^2. \tag{15}$$

The corresponding temperature spectrum $\lambda_n^{(\beta)}$ is of the form

$$\lambda_n^{(\beta)}=[\pi(2n+1)/\beta]^2+\Delta^2+e\mu H+p_x^2,\quad -\infty<n<\infty. \tag{16}$$

We note that in contrast to the case $H=0$, the quantity $|p_x|$ lies outside of the interval of $eH\beta$ (15).

In the opposite limiting case of strong fields (low temperatures), when

$$(p_x-eH\tau)^2\gg eH,\ \Delta^2,\ \lambda_n, \tag{17}$$

the integrability condition calls for the vanishing of Φ_n as $\tau\to\infty$. The spectrum of (14) is then equivalent to the spectrum in the Landau problem of an electron in a magnetic field, subject to satisfaction of the standard inequality

$$|p_x-eH\tau|<eH\beta, \tag{18}$$

which determines the degree of degeneracy of the energy levels with respect to p_x. Thus, in the region (17), (18) we have

$$\lambda_n^{(H)}=(2n+1+\mu)eH+\Delta^2,\quad 0\leqslant n<\infty,\quad \mu=\pm1. \tag{19}$$

We note that in real time the inequality (18) means that pair production by an electric field takes place after a finite time interval, and outside this interval the field only accelerates the pairs.[26]

At $T\neq0$ the parameter p_x in the last case varies in a limited interval determined by the inequalities (17) and (18). Therefore at $T=0$ the state density turns out to be a function of p_x, even though the spectrum (19) does not depend on p_x.

Using the form of the spectrum of Eq. (14) in various asymptotic regions of the values of T and H, we present explicit expressions for $\zeta(s)$.

In regions (15)

$$\frac{1}{\beta L}\zeta^{(\beta)}(s)=\frac{2}{\beta}\sum_{n=-\infty}^{\infty}2\int_{\alpha_\beta eH\beta}^{\infty}\frac{dp_x}{2\pi}\left\{\left[\frac{\pi}{\beta}(2n+1)\right]^2+\Delta^2+e\mu H+p_x^2\right\}^{-s}, \tag{20}$$

where α_β is a constant of the order of unity. Integrating with respect to p_x, we obtain

$$\frac{1}{\beta L}\zeta^{(\beta)}(s)\approx\frac{1}{\beta\pi^{1/2}}\frac{\Gamma(s-{}^1/{}_2)}{\Gamma(s)}\sum_{n=-\infty}^{\infty}\left\{\left[\frac{\pi}{\beta}(2n+1)\right]^2+\Delta^2+e\mu H\right\}^{1/2-s}$$
$$-\alpha_\beta\frac{2eH}{\pi}\sum_{n=-\infty}^{\infty}\left\{\left[\frac{\pi}{\beta}(2n+1)\right]^2+\Delta^2+e\mu H\right\}^{-s}. \tag{21}$$

The second term in (21) and the contribution of the term $e\mu H$ in the first term describes small "field" increments to $\zeta(s)$. This means that the summation over $\mu=\pm1$ must be carried out only when the corrections are calculated.

In the region of values of the parameters H and T $(eH\beta^2\gg1)$, the state density $\nu(p_x)$ is, according to inequalities (17) and (18),

$$\nu(p_x)=L\beta\frac{eH}{\pi}\left\{1-\alpha_H\frac{2}{eH\beta}[2eH(n+1)+\Delta^2]^{1/2}\right\} \tag{22}$$

(α_H is a constant of the order of unity), and $\zeta^{(H)}(s)$ takes the form

$$\frac{1}{\beta L}\zeta^{(H)}(s)\approx\frac{eH}{2\pi}\sum_{\mu=\pm1}\sum_{n=0}^{n_{max}}\left\{1-\alpha_H\frac{2}{eH\beta}\right.$$
$$\left.\times[2eH(n+1)+\Delta^2]^{1/2}\right\}\{eH(2n+1)+\Delta^2+e\mu H\}^{-s}, \tag{23}$$

where $n_{max}\sim eH\beta^2\gg1$. We shall hereafter assume the upper limit of the sum over n (23) in the principal approximation in $(eH\beta^2)^{-1}\ll1$ to be infinity. In analogy with (21), the second term in (23) determines small temperature corrections to the principal field contribution to $\zeta(s)$.

BEHAVIOR OF PD IN STRONG FIELDS (AT LOW TEMPERATURES)

We investigate first in detail the case of zero temperature (23). In this limit, the sum over n can be calculated exactly:

$$\frac{1}{\beta L}\zeta^{(H)}(s)=\frac{eH}{2\pi}(2eH)^{-s}\left\{\zeta\left(s,\frac{\Delta^2}{2eH}\right)-\left(\frac{\Delta^2}{2eH}\right)^{-s}\right\}, \tag{24}$$

where

$$\zeta(s,a)=\sum_{n=0}^{\infty}(n+a)^{-s}$$

is the generalized Riemann ζ function (see, e.g., Ref. 27).

Using the known properties of $\zeta(s,a)$ we obtain

$$\frac{1}{\beta L}\zeta^{(H)}(0)=-\frac{\Delta^2}{\pi}, \tag{25}$$

$$\frac{1}{\beta L}\zeta^{(H)\prime}(0)=\frac{eH}{\pi}\left\{\frac{\Delta^2}{eH}\ln(2eH)+\ln\frac{\Delta^2}{2eH}+2\ln\Gamma\left(\frac{\Delta^2}{2eH}\right)-\ln 2\pi\right\}. \tag{26}$$

As a result, the expression (6) for V_{eff} takes the form

$$V_{eff}=\frac{\Delta^2}{g^2}+\frac{\Delta^2}{2\pi}\ln 2eH+\frac{eH}{2\pi}\ln\frac{\Delta^2}{2eH}+\frac{eH}{\pi}\ln\Gamma\left(\frac{\Delta^2}{2eH}\right)-\frac{eH}{2\pi}\ln 2\pi-\frac{\Delta^2}{2\pi}\ln c_R^2. \tag{27}$$

The equilibrium value of the order parameter $\Delta(H)$ is determined from the condition that the effective potential be a minimum:

$$\left.\frac{\partial^2 V_{eff}}{\partial\Delta^2}\right|_{\Delta=\Delta(H)}>0,\quad \left.\frac{\partial V_{eff}}{\partial\Delta}\right|_{\Delta=\Delta(H)}=0. \tag{28}$$

The constant c_R, using the normalization[11]

$$\left.\frac{\partial^2 V_{eff}}{\partial\Delta^2}\right|_{\Delta=\Delta_0}=2g^{-2},\quad H=0 \tag{29}$$

can be easily connected with the gap Δ_0 in the absence of a field:

$$\Delta_0=c_R\exp\{-\pi\hbar v_F/g^2\}. \tag{30}$$

The conditions (28) express the fact that V_{eff}, by definition, is extremal with respect to variations of Δ. Indeed, $V_{eff}=-\mathscr{L}'(\Delta,E)$, where $\mathscr{L}'$ is an increment, due to the polarization of the medium, to the Lagrangian density of the electromagnetic field (see, e.g., Ref. 28), while the last expression in (28) is simply the "equation of motion" for the field Δ. The renormalization condition (29) calls for certain comments. Our scheme for calculating the ground state agrees in its idea with the scheme used in quantum electrodynamics.[28] There is, however, a difference connected with the renormalization procedure. In PD (see also Ref. 17), the gap in the spectrum is not a specified quantity, but is obtained from the condition that the energy be a minimum. Therefore the natural physical condition for the renormalization of V_{eff} is a fixed equilibrium $\Delta=\Delta_0$ in a zero field. For the investigated model, all the remaining quantities are then fully defined.[17] In this respect there is a qualitative difference from quantum electrodynamics[28] where the renormalization reduces to a fixing of the physical charge, and allowance for the polarization of the vacuum leads only to corrections, nonlinear in E^2, to the Lagrangian of the electromagnetic field.

Substituting (30) in (27), we obtain V_{eff} as a function of Δ and H:

$$V_{eff}=\frac{\Delta^2}{2\pi}\left\{\ln\frac{2eH}{\Delta_0^2}+\frac{eH}{\Delta^2}\ln\frac{\Delta^2}{2eH}+\frac{2eH}{\Delta^2}\left[\ln\Gamma\left(\frac{\Delta^2}{2eH}\right)-\frac{1}{2}\ln 2\pi\right]\right\}. \tag{31}$$

Equation (31) is the final result, in which it is necessary to return to the (x,t) space by making the substitution $H\to -iE$. Separating the real and imaginary parts of V_{eff} and restoring the dimensionality, we have

$$\mathrm{Re}\,V_{eff}=\frac{\Delta^2}{2\pi\hbar v_F}\left\{\ln\frac{2eE\xi_0}{\Delta_0}+\frac{2eE\xi_0\Delta_0}{\Delta^2}\times\mathrm{Im}\ln\Gamma\left(1+i\frac{\Delta^2}{2eE\xi_0\Delta_0}\right)-\frac{\pi eE\xi_0\Delta_0}{2\Delta^2}\right\}, \tag{32}$$

$$\mathrm{Im}\,V_{eff}=\frac{eE}{2\pi}\ln\left\{1-\exp\left(-\frac{\pi\Delta^2}{eE\xi_0\Delta_0}\right)\right\}. \tag{33}$$

The self-consistency equation $\partial\,\mathrm{Re}\,V_{eff}/\partial\Delta=0$ determines the function $\Delta(E)$:

$$\ln\frac{\Delta_0}{2eE\xi_0}=\mathrm{Re}\,\Psi\left(1+i\frac{\Delta^2}{2eE\xi_0\Delta_0}\right) \tag{34}$$

(Ψ is the logarithmic derivative of the Γ function).

Equation (34) was first obtained (by another method) in Ref. 23, where it was concluded that a critical phase-transition field exists

$$\Delta(E_c)=0,\quad E_c=\frac{1}{2}\Delta_0 e^C/e\xi_0,$$

where C is the Euler constant. The presence of $\mathrm{Im}\,V_{eff}$ [Eq. (33)], however, makes it possible to consider the polarization $\Delta(E)$ of the PD only at $\mathrm{Im}\,V_{eff}\ll\mathrm{Re}\,V_{eff}$. Actually, the imaginary part of the effective potential determines the characteristic lifetime of the system.[22] Naturally, it is meaningful to speak of equilibrium properties only when this time is long, i.e., when the condition that $\mathrm{Im}\,V_{eff}$ be small is satisfied. At the same time, as $E\to E_c$ the gap vanishes ($\Delta\to 0$) and $\mathrm{Im}\,V_{eff}\to -\infty$, while the lifetime of the system $\tau=-2/\mathrm{Im}\,V_{eff}$ tends to zero.

The very concept of a PD in a field E is meaningful so long as the notion of the gap in the spectrum is valid, i.e., up to fields $E\lesssim E_0<E_c$, where E_0 is obtained from the condition

$$\mathrm{Re}V_{eff}(\Delta(E_0),E_0)=\mathrm{Im}V_{eff}(\Delta(E_0),E_0). \tag{35}$$

Therefore the formal conclusion of the existence of a phase transition, obtained from an analysis of $\mathrm{Re}\,V_{eff}$ only, is not valid, because of the intense production of pairs of free carriers, while the transition into the metallic state is smooth, without singularities in the kinetic coefficients. A consequence of the condition (35) should be the vanishing of the high-frequency absorption peak of the PD at $E\sim E_0$ [of the order of 10^5 V/cm for $(CH)_x$] and the simultaneous appearance of the plasma edge that is typical of metals.

It is clear from the foregoing analysis that it is meaningful to speak of a PD and of the polarization of its ground state $\Delta=\Delta(E)$ by an electric field only at small E ($eE\xi_0\ll\Delta_0$), when the particle production is exponentially suppressed:

$$\mathrm{Im}\,V_{eff}=-\frac{eE}{2\pi}\exp\left(-\frac{\pi\Delta_0}{eE\xi_0}\right); \tag{36}$$

in this case

$$\Delta(E)\approx\Delta_0\left\{1-\frac{1}{6}\left(\frac{eE\xi_0}{\Delta_0}\right)^2\right\}. \tag{37}$$

We recall the connection between $\mathrm{Im}\,V_{eff}$ with the density of the produced particles. The square of the modulus of the vacuum-vacuum amplitude is (see, e.g., Ref. 26)

$$|\langle 0_-|0_+\rangle|^2=\exp\{2\mathrm{Im}V_{eff}L\tilde{t}\}, \tag{38}$$

where $|0_\pm\rangle$ are the vacuum states as $t\to\pm\infty$, and $\tilde{t}$ is the time interval during which the field acts. Let n_p be the probability of production of a pair of carriers in the state p. The probability that not a single pair is produced during the entire of action of the field E is

$$\prod_p (1-n_p)=\exp\sum_p \ln(1-n_p)=\exp\left\{\frac{L}{2\pi}2\int dp_x \ln(1-n_p)\right\}.$$

Recognizing that the p_x interval that is essential for particle production is finite [see (18)] and assuming n_p to be independent of the momentum, as is confirmed by direct calculation,[26] we have

$$\prod_p (1-n_p)=\exp\left\{\frac{L\tilde{t}}{\pi}eE\ln(1-n)\right\}. \quad (39)$$

Comparing (39) with (38) and (33) we obtain

$$n=\exp(-\pi\Delta^2/eE\Delta_0\xi_0),$$

and for the intensity of particle production (per unit length and unit time) we have

$$I_{e-h}=\frac{2}{\tilde{t}L}\int\frac{dp_x}{2\pi}n_p=\frac{eE}{\pi\hbar}\exp\left(-\frac{\pi\Delta^2}{eE\Delta_0\xi_0}\right). \quad (40)$$

Equation (40) coincides with the results of Ref. 11 for the one-dimensional problem at equal masses of the electrons and holes.

We return now to expression (32) where Re V_{eff}. It is easy to write with its aid an expression for the induction D ($E \ll E_c$) (Ref. 28):

$$D=E-4\pi\rho_f\frac{\partial \operatorname{Re} V_{eff}}{\partial E}, \quad (41)$$

where ρ_f is the density of the one-dimensional chains in the sample. The appearance of ρ_f in (41) is due to the three-dimensional penetration of the field into the sample. From (41) and (32) follows directly the standard expression for the dielectric constant of a PD in the linear-response limit[16]:

$$\varepsilon_0=1+{}^1/_6(\hbar\omega_p/\Delta_0)^2, \quad (42)$$

where $\omega_p^2=4\pi e^2 n\rho_f/m$ is the square of the plasma frequency, $mv_F=\pi n/2$, n is the linear density of the conduction electrons. For the parameters of polyacetylene we have $\varepsilon_0\approx 15$, which correlated well with the experimental data.[6]

ROLE OF TEMPERATURE EFFECTS

We consider now the temperature corrections to (24). The expression for the temperature increment to $\zeta^{(H)}(s)$ is of the form

$$\frac{1}{\beta L}\delta\zeta^{(H)}(s)=-\frac{\alpha_H}{\pi\beta}(2eH)^{1/2-s}$$

$$\times\sum_{n=0}^{\infty}\{(n+1+\bar{q})^{1/2-s}-(n+1+\bar{q})^{1/2}(n+\bar{q})^{-s}\},\quad \bar{q}=\frac{\Delta^2}{2eH}. \quad (43)$$

At arbitrary $\bar{q}$ it is impossible to evaluate exactly the sums in (43). We confine ourselves therefore to calculation of the asymptotic values in two limiting regions, $\bar{q}\gg 1$ and $\bar{q}\ll 1$ (the details of the calculations are relegated to the Appendix). For $\bar{q}\gg 1$ we have

$$\operatorname{Re}\delta V_{eff}\approx\frac{\alpha_H}{\pi\beta}\Delta\left\{\ln\left(\frac{\Delta_0}{\Delta}\right)^2+\frac{2\pi\hbar v_F}{g^2}\right\}(\hbar v_F)^{-1}, \quad (44)$$

$$\operatorname{Im}\delta V_{eff}\approx-\frac{2\alpha_H}{3\pi\beta}\frac{\Delta^3(\hbar v_F)^{-1}}{eE\xi_0\Delta_0}\left[\ln\left(\frac{\Delta_0}{\Delta}\right)^2+\frac{2\pi\hbar v_F}{g^2}\right]$$
$$-\frac{4\alpha_H}{9\pi\beta}\frac{\Delta^3}{eE\xi_0\Delta_0}(\hbar v_F)^{-1}. \quad (45)$$

It is seen from the foregoing equations that

$$\operatorname{Re}\delta V_{eff}\ll\operatorname{Im}\delta V_{eff},$$

i.e., the temperature influences mainly the pair-generation process. In the case $\bar{q}\ll 1$ we have

$$\operatorname{Re}\delta V_{eff}\approx-4{,}35\alpha_H(\pi\beta)^{-1}(eE/\hbar v_F)^{1/2}\cdot\ln(2eE\xi_0/\Delta_0),$$
$$\operatorname{Im}\delta V_{eff}=-\operatorname{Re}\delta V_{eff}. \quad (46)$$

In the other limiting case, $E=0$ and $T\neq 0$ (cf. Ref. 25) we have

$$\frac{1}{\beta L}\zeta^{(\beta)}(s)=\frac{1}{2\beta^2}\left(\frac{2\beta}{\pi}\right)^{2s}\frac{\Gamma^2(s-{}^1/_2)s(2s-1)}{\Gamma(2s+1)}$$
$$\times\left\{D\left(s-{}^1/_2,\frac{\beta\Delta}{\pi}\right)-2^{1-2s}D\left(s-{}^1/_2,\frac{\beta\Delta}{2\pi}\right)\right\}, \quad (47)$$

$$D(s,a)=2\sum_{n=1}^{\infty}(n^2+a^2)^{-s}. \quad (48)$$

Using the regular representation of the function D (see the Appendix) we obtain

$$\frac{1}{\beta L}\zeta^{(\beta)}(0)=-\frac{\pi}{2\beta^2}\left(\frac{\beta\Delta}{\pi}\right)^2. \quad (49)$$

An expression for $\zeta^{(\beta)\prime}(0)$ can be obtained in explicit form in the limit of high ($\beta\Delta\ll 1$) and low ($\beta\Delta\gg 1$) temperatures. At low temperatures

$$\frac{1}{\beta L}\zeta^{(\beta)\prime}(0)\approx\frac{\pi}{\beta^2}\left(\frac{\beta\Delta}{\pi}\right)^2\left\{\ln\Delta-\frac{1}{2}\right\}, \quad (50)$$

and at high temperatures

$$\frac{1}{\beta L}\zeta^{(\beta)\prime}(0)\approx\frac{\pi}{\beta^2}\left\{\left(\frac{\beta\Delta}{\pi}\right)^2\ln\frac{\pi}{\beta}+\Psi(1)\left(\frac{\beta\Delta}{\pi}\right)^2+\frac{7\zeta(3)}{16}\left(\frac{\beta\Delta}{\pi}\right)^4\right\}. \quad (51)$$

Here $\Psi(1)=-C$ is the Euler constant, and $\zeta(3)\approx 1.202$. From (48), (49), and the expression for V_{eff} we get

$$V_{eff}(\beta\Delta\gg 1)\approx\frac{\Delta^2}{2\pi\hbar v_F}\left\{\ln\left(\frac{\Delta}{\Delta_0}\right)^2-1\right\}$$

it is easy to obtain an equation for the equilibrium gap at $T=0$, which naturally coincides with (30).

The minimum of V_{eff} determines the equilibrium value of $\Delta(T)$. It is easy to verify that the expansion of V_{eff} at $\beta\Delta\ll 1$ coincides exactly with the free-energy functional of the PD in the Ginzburg-Landau form:

$$V_{eff}(\beta\Delta\ll 1)=\frac{\Delta^2}{2\pi\hbar v_F}\left\{\ln\frac{T}{T_c}+\frac{7\zeta(3)}{16}\left(\frac{\Delta}{\pi T}\right)^2\right\},\quad T_c=\frac{\Delta_0}{\pi}e^C. \quad (52)$$

From this follows formally the existence of a critical temperature T_c of the second-order phase transition, at which the gap Δ vanishes.[1]

As noted in the introduction, the thermodynamics of a one-dimensional PD should be constructed from the very outset in terms of stable states—solitons. We note, however, that the interactions of chains can lead at certain temperatures to a decay of one-dimensional solitons and by the same token to restoration of the electronic systematics of the states in the PD.

We proceed now to consider the field corrections to the free energy of the PD, recalling that the thermodynamic approach has a limited applicability if an electric field is present in the system. For the field correction in (21) we have

$$\frac{1}{\beta L}\delta\zeta^{(\beta)}(s)\approx i\frac{2\alpha_\beta eE}{\pi}\left(\frac{\pi}{\beta}\right)^{-2s}\sum_{\mu=\pm1}\left\{D\left(s,\frac{\beta}{\pi}(\Delta^2+ieE\mu\hbar v_F)^{1/2}\right)\right.$$
$$\left.-2^{-2s}D\left(s,\frac{\beta}{\pi}(\Delta^2+ieE\mu\hbar v_F)^{1/2}\right)\right\}. \quad (53)$$

Using the properties of the D functions (see the Appendix), we can find that

$$\frac{1}{\beta L}\delta\zeta^{(\beta)}(0)=0, \quad (54)$$

$$\frac{1}{\beta L}\delta\zeta^{(\beta)\prime}(0)=-i\frac{2\alpha_\beta eE}{\pi}\sum_\mu \ln\left[2\,\mathrm{ch}\left(\frac{\beta\Delta}{2}\left(1+i\mu\frac{eE\hbar v_F}{\Delta^2}\right)^{1/2}\right)\right]. \quad (55)$$

We note that according to the inequalities (15), the radicand in (53) must be expanded in powers of $eE\hbar v_F/\Delta^2$. It is clear that the summation over $\mu=\pm1$ in (53) leaves only odd powers of E, i.e., the field correction (55) determines the imaginary increment to the free energy of the system:

$$\mathrm{Im}\,\delta V_{eff}=-\frac{8\alpha_\beta eE}{\pi}\ln\left[2\,\mathrm{ch}\frac{\beta\Delta}{2}\right]. \quad (56)$$

The main effect of the field in the indicated temperature region reduces to the appearance of a current in the system and to a weak (because of the small imaginary part of the free energy) distortion of the equilibrium distribution of the particles.

Let us analyze expression (56), which allows us to determine the density of the particles taken out of the thermodynamic-equilibrium state by the external field. It is easily seen that Im δV_{eff} is proportional to the free energy of a one-dimensional harmonic oscillator of frequency Δ with Fermi filling of the energy levels. Therefore the linear density of the nonequilibrium particles (with energies in the interval $[\Delta, (\Delta^2+p_c^2)^{1/2}]$, where $p_c=\alpha_\beta eE\beta\hbar V_F\ll\Delta$) is equal to the probability of observing a particle with energy $(\Delta^2+p_x^2)^{1/2}$, $(-p_c<p_x<p_c)$, integrated over the phase volume

$$\bar N_n=4\int_0^{p_c}\frac{dp_x}{2\pi}(\exp[\beta(\Delta^2+p_x^2)^{1/2}]+1)^{-1}\approx\frac{2\alpha_\beta}{\pi}eE\beta(1+e^{\beta\Delta})^{-1}. \quad (57)$$

The inequality $eE\beta^2\ll1$ makes $\bar N_n$ always smaller than the equilibrium density of the carrier pairs, and the influence of the nonequilibrium group of particles on the thermodynamics of the system can be neglected. In other words, this means that the average time $\tau=-2/\mathrm{Im}\,V_{eff}$ that the system remains in a thermodynamic-equilibrium state is long.

We conclude this section with a few words concerning the numerical coefficients α_β and α_H, which appear in the calculations of the field and temperature corrections to V_{eff}. Usually such coefficients are determined by matching together the asymptotic solutions in the intermediate region. In our case, however, such a matching is impossible both from the formal mathematical point of view and from the physical. Indeed, owing to the strong nonstationarity, in the region where the characteristic energy of the pair in the field becomes equal to the temperature one cannot speak of equilibrium thermodynamics. Therefore the values of α_β and $\alpha_H\sim1$ cannot be determined exactly in our approach and they must be found from a solution of the kinetic equation in the intermediate region.

CONCLUSION

We discuss now briefly the possible manifestations of the instability of a PD in an electric field. In the presence of free electrons (holes) in the band, small fluctuations of the lattice, with $q=2k_F$, become unstable and this leads in final analysis to formation of strongly coupled electron-lattice states—solitons and polarons. The polaron of the Gross-Neveau model has an energy $E_p=2^{3/2}\Delta_0/\pi$ (Ref. 13) and carries a charge $\pm|e|$, and a spin 1/2, whereas the charged solitons have no spin.[6] Simple estimates show that in strong fields $\alpha^2E_c\ll E<E_c$ the characteristic time $t_L\sim\lambda^{-1/2}/\omega(2k_F)$ of the small lattice fluctuation is sufficient for the tunnel-produced electron-hole pair to become separated far enough from each other to make energywise possible the formation of only e and h polarons. The current carriers in strong fields are therefore apparently the polarons, and an increase of the conductivity should be accompanied by an increase of the Pauli magnetic susceptibility. In the case of weak fields, $E\lesssim\alpha^2E_c$, direct production of charged soliton-antisoliton pairs should take place. The probability of this process is additionally suppressed (the solitons are heavy) compared with the production of e–h pairs, and this decreases the conductivity substantially. A detailed analysis of this group of problems requires a separate investigation.

We have described above the picture that can take place at low temperatures $eE\beta^2\gg1$. At high temperatures $eE\beta^2\ll1$ the carriers in the PD are thermally activated spinless solitons.

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APPENDIX

We present here a brief derivation of the equations needed to work with temperature D-functions (50) and not found in the handbook literature:

$$D(s,a)=\sum_{n=1}^{\infty}(n^2+a^2)^{-s}. \quad (A1)$$

To obtain the expressions in the main text, we need to know $D'(0,a)$, $D(-1/2,a)$, and $D(0,a)$. We therefore obtain for $D(s,a)$ a representation that is valid, in contrast to (A1), also for Re $s<1$. Recognizing that the D functions are universal in all thermodynamic calculations by the generalized ζ-function $\zeta(s)$ method, we present two different regular representations of (A1) (in analogy with the known representations of Hermite and Riemann for the Riemann ζ function[27]).

REPRESENTATION OF D IN THE HERMITE FORM

For this purpose[25] we use the known Abel-Plana formula[27] in the form

$$\sum_{n=1}^{\infty} f(n)=\frac{1}{2}f(1)+\int_1^{\infty} f(\tau)\,d\tau-i\int_0^{\infty}\frac{f(1+it)-f(1-it)}{e^{2\pi t}-1}\,dt \tag{A2}$$

as applied to (A1) we have

$$D(s,a)=(1+a^2)^{-s}+a^{-2s}\left[B\left(\frac{1}{2},s-\frac{1}{2}\right)-2\int_0^{1/a}d\tau\,(1+\tau^2)^{-s}\right]$$
$$+4\int_0^{\infty}\frac{dt}{e^{2\pi t}-1}\,\frac{1}{[(1+a^2-t^2)^2+4t^2]^{s/2}}\sin\left(s\,\mathrm{arctg}\frac{2t}{1+a^2-t^2}\right). \tag{A3}$$

Equation (A3) is regular in the entire range of s, with the exception of the points $s=1/2-n$ $(n=0, 1, 2, \ldots)$. The calculations yield

$$D(0,a)=-1, \tag{A4}$$

$$D'(0,a)=-2\ln\left\{\frac{2\,\mathrm{sh}\,\pi a}{a}\right\}. \tag{A5}$$

Expressions (A4) and (A5) are used to calculate the corrections (53). The functions $D(-1/2,a)$ and $D'(-1/2,a)$ are needed to find $\zeta^{\beta}(0)$ in (47) and are singular. In the equations for $\zeta^{\beta}(0)$ and $\zeta^{\beta'}(0)$, the singularities cancel out and the answer is determined by the asymptotic forms of the regular parts of the function (A3) at $s=-1/2$. Their calculation entails no particular difficulty [Eqs. (50) and (51)].

REPRESENTATION OF THE D FUNCTION IN THE RIEMANN FORM

Using the Riemann transformation, we represent (A1) in the form

$$D(s,a)=\frac{2}{\Gamma(s)}\int_0^{\infty}dx\,x^{s-1}\sum_{n=1}^{\infty}e^{-n^2x}=\frac{1}{\Gamma(s)}\int_0^{\infty}dx\,x^{s-1}\left\{\theta_3\left(0\,\middle|\,\frac{ix}{\pi}\right)-1\right\}. \tag{A6}$$

Here $\theta_3(z\,|\,\tau)$, and θ is the Jacobi function. The integral (A6) converges at $\mathrm{Re}\,s>1/2$, and to calculate $D(0,a)$ and $D'(0,a)$ it is necessary to regularize (A6). To this end we transform $\theta_3(z\,|\,\tau)$, using the imaginary Jacobi transformation[27]:

$$\theta_3\left(\frac{z}{\tau}\,\middle|\,-\frac{1}{\tau}\right)=(-i\tau)^{1/2}\exp\left(\frac{i\pi z^2}{\tau}\right)\theta_3(z|\tau). \tag{A7}$$

Using (A7) we have

$$D(s,a)=\frac{1}{\Gamma(s)}\int_0^{\infty}dx\,x^{s-1}\exp(-a^2x)\left(\left(\frac{\pi}{x}\right)^{1/2}-1\right)$$
$$+\frac{4\pi^{1/2}}{\Gamma(s)}\left(\frac{\pi}{a}\right)^{s-1}\sum_{n=1}^{\infty}n^{s-1/2}K_{s-1/2}(2\pi an), \tag{A8}$$

where $K_\nu(z)$ is a Macdonald function. Introducing the incomplete gamma functions $\gamma^*(s,x)$ and $\Gamma(s,x)$ (see Ref. 27)

$$\gamma^*(s,x)=\frac{x^{-s}}{\Gamma(s)}\int_0^x dt\,e^{-t}t^{s-1},\quad \Gamma(s,x)=\int_x^{\infty}dt\,e^{-t}t^{s-1}, \tag{A9}$$

which are regular for all s and x, we obtain

$$D(s,a)=-\gamma^*(s,a^2)+\frac{\Gamma(s-1/2)}{\Gamma(s)}\pi^{1/2}\gamma^*(s-1/2,a^2)-a^{-2s}\frac{\Gamma(s,a^2)}{\Gamma(s)}$$
$$+\pi^{1/2}a^{-2(s-1/2)}\frac{\Gamma(s-1/2,a^2)}{\Gamma(s)}+\frac{4\pi^s}{\Gamma(s)}a^{1/2-s}\sum_{n=1}^{\infty}n^{s-1/2}K_{s-1/2}(2\pi an). \tag{A10}$$

Since a Macdonald function of half-integer index reduces to exponentials, the series we need $(s=0)$ can be easily calculated. Calculations with the aid of (A10) yield a result that coincides with (A4) and (A5).

We determine now the sums of the numerical series that arise in the calculation of the asymptotic form of the second term in Eq. (43) at $\bar{q}\ll 1$

$$J(\bar{q})=(2eH)^{1/2-s}\sum_{n=0}^{\infty}\frac{(n+\bar{q}+1)^{1/2}}{(n+\bar{q})^s}, \tag{A11}$$

$$J(\bar{q}\ll 1)\approx(2eH)^{1/2-s}\left\{\bar{q}^{-s}+\frac{1}{2}\bar{q}^{1-s}+\rho(s)-s\bar{q}\rho(s+1)+\frac{\bar{q}}{2}\sigma(s)\right\}, \tag{A12}$$

$$\rho(s)=\sum_{n=1}^{\infty}n^{-s}(n+1)^{1/2},\quad \sigma(s)=\sum_{n=1}^{\infty}n^{-s}(n+1)^{-1/2}. \tag{A13}$$

It follows from (A12) and (A13) that

$$\frac{1}{\beta L}\delta\zeta^{(H)}(0)\approx-\alpha_H\frac{(2eH)^{1/2}}{\pi\beta}\left\{\zeta(-1/2)+\frac{1}{2}\bar{q}\zeta(1/2)+1+\rho(0)+\frac{\bar{q}}{2}[1+\sigma(0)]\right\};$$
$$\frac{1}{\beta L}\delta\zeta^{(H)\prime}(0)\approx-\alpha_H\frac{(2eH)^{1/2}}{\pi\beta}\left\{-\ln(2eH)\left[\zeta(-1/2)+\frac{\bar{q}}{2}\zeta(1/2)\right]\right.$$
$$+\zeta'(-1/2)-\bar{q}[\zeta(1/2)-1/2\zeta'(1/2)]-\ln(2eH)\left[1+\rho(0)+\frac{\bar{q}}{2}(1+\sigma(0))\right. \tag{A14}$$

$$\left.-\left(1+\frac{\bar{q}}{2}\right)\ln\bar{q}+\rho'(0)-\bar{q}\left[\rho(1)-\frac{1}{2}\sigma'(0)\right]\right\}. \tag{A15}$$

Regularizing the series with the aid of the Abel-Plana formula, we obtain

$$A=1+\rho(0)+\zeta(-1/2)\approx-4.35;\quad B=1+\sigma(0)+\zeta(1/2)\approx1.02;$$
$$C=\rho'(0)+\zeta'(-1/2)\approx-3.26;\quad D=\zeta'(1/2)+\sigma'(0)-2\rho(1)-2\zeta(1/2)\approx-10.34, \tag{A16}$$

i.e., δV_{eff} at $\bar{q}\ll 1$ [cf. (44) and (45)] is equal to

$$\delta V_{\mathrm{eff}}\approx-\alpha_H\frac{(2eH)^{1/2}}{\pi\beta}\left\{\left(A+\frac{\bar{q}}{2}B\right)\ln\frac{\Delta_0^2}{2eH}+C\right.$$
$$\left.-\left(1+\frac{\bar{q}}{2}\ln\bar{q}\right)+\frac{\bar{q}}{2}D+\frac{2\pi}{g^2}\left(A+\frac{\bar{q}}{2}B\right)\right\}.$$

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